Rheology of granular mixtures under uniform shear flow: Enskog kinetic theory versus molecular dynamics simulations

José María Montanero*
Departamento de Electrónica e Ingeniería Electromecánica, Universidad de Extremadura, E-06071 Badajoz, Spain

Vicente Garzó†
Departamento de Física, Universidad de Extremadura, E-06071 Badajoz, Spain

Meheboob Alam‡
Engineering Mechanics Unit, Jawaharlal Nehru Center, Jakkur P.O., Bangalore 560064, India

Stefan Luding§
Particle Technology, DelftChemTech, Julianalaan 136, 2628 BL Delft, The Netherlands
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The rheological properties for dilute and moderately dense granular binary mixtures of smooth, inelastic hard disks/spheres under uniform shear flow in steady state conditions are reported. The results are based on the Enskog kinetic theory, numerically solved by a dense gas extension of the Direct Simulation Monte Carlo method for dilute gases. These results are confronted to the ones also obtained by performing molecular dynamics simulations with very good agreement for the lower densities and higher coefficients of restitution. It appears that the range of densities for which the Enskog equation applies decreases with increasing dissipation.

I. INTRODUCTION

Rapid granular flows can be well modeled by an idealized system of smooth hard disks/spheres with inelastic collisions [1, 2]. Despite the simplicity of the model, it has been widely studied in the last few years as a prototype to gain some insight into the "microscopic" understanding of physical mechanisms involved in granular flows. One well established tool is the kinetic theory and, more specifically, the Boltzmann equation for a low density gas [3, 4, 5, 6].

In recent years, some methods have been developed to solve it and get accurate predictions over a wide range of parameters. For finite higher densities, the Enskog kinetic equation [7, 8] can be considered as the extension of the Boltzmann equation. As for elastic collisions, the inelastic Enskog equation takes into account spatial correlations through the pair correlation function but neglects the effect of correlations between the velocities of two particles that are about to collide (molecular chaos assumption). Nevertheless, some deviations from molecular chaos have been observed in molecular dynamics (MD) simulations of granular fluids in driven, sheared, or homogeneous states [9, 10, 11, 12, 18]. Being not significant for dilute systems [13], the velocity correlations increase with the density. Although the presence of these correlations restricts the range of validity of the Enskog equation, it can still be considered as a good approximation at moderate densities since, for instance, the Enskog kinetic theory [8] successfully models the hydrodynamic profiles obtained in recent NMR experiments on a three-dimensional vibrofluidized granular medium [14] or from simulations for a two-dimensional system, even at very high densities [15].

Most of the comparisons carried out between kinetic theory results, molecular dynamics (MD) and especially hard sphere event-driven (ED) simulations have been devoted to monodisperse systems, where all the grains have the same mass and size. Needless to say, a real granular system is usually characterized by some degrees of polydispersity in mass and size, which can lead to segregation in an otherwise homogeneous mixture. As kinetic theory predicts for the homogeneous state [16, 17, 18, 19], MD simulations [20, 21] show that the kinetic temperatures for each species are clearly different and present a complex dependence on the parameters of the problem (dissipation, mass ratio, size ratio, composition, and density). Good agreement for the temperature ratio between Enskog theory and simulations is found for moderate densities and not too strong dissipation [20].

*E-mail: jmm@unex.es
†E-mail: vicenteg@unex.es
‡E-mail: meheboob@jncasr.ac.in
§E-mail: s.luding@tnw.tudelft.nl

In the case of shearing flow states, recent MD simulations have been performed [22, 23] to analyze the (bulk) rheological properties of granular mixtures under uniform shear flow (USF) conditions. Numerical results for the shear stress and the granular energy were compared with those derived from a kinetic theory valid in the low dissipation limit [24, 25]. The comparison between theory and simulation shows an excellent agreement in the quasielastic limit even at large size disparities. Given that this theory [24, 25] only applies for weak inelasticity, it assumes energy equipartition and the granular temperature coincides with the partial temperatures of each species. However, beyond the low-dissipation limit, the failure of energy equipartition in granular fluids has not only been predicted by numerical "experiments" [18, 19, 20, 21] but also was observed in real experiments [26].

The goal of this paper is to determine the rheological properties of a granular binary mixture under USF conditions in the context of the Enskog kinetic theory, and to compare the theory to ED simulations. The USF is characterized by uniform density and temperature and a constant velocity profile. In contrast to classical, elastic fluids, a steady state is reached in the system when the continuous loss of energy due to inelastic collisions is compensated for by the viscous (shear) heating. As a consequence, for a given shear rate, the granular temperature as well as the rheological properties are functions of the coefficients of restitution.

Two special situations allow for simple analytical results. First, in the low density limit the corresponding Boltzmann equation can be approximately solved by Grad's method [27]. This solution compares quite well with Monte Carlo simulations [27, 28, 29], even for strong dissipation. Second, for small shear rates but finite densities, the Enskog equation can be solved by the Chapman-Enskog method [30] and an explicit expression for the Navier-Stokes shear viscosity coefficient has been obtained in the leading Sonine approximation [31]. It must be remarked that the kinetic theory derived in Ref. [31] differs from the one previously obtained in Refs. [24] and [25] since the former should apply for an arbitrary degree of dissipation and takes into account the effect of temperature differences on momentum transport. Beyond the above two special cases (dilute gas and Navier-Stokes approximation), Lutsko [32] has recently solved the Enskog equation for a moderately dense mixture under USF by using a generalized moment method. Although this theory compares quite well with MD simulations, it appears too complicated to be useful for practical purposes here, since it involves many different collision integrals that must be solved numerically. Instead, as an alternative to the above theory [32], we compute the rheological properties from a *numerical* solution of the Enskog equation by means of an extension of the well-known Direct Simulation Monte Carlo (DSMC) method [33] to dense gases [34, 35, 36].

Given that MD simulation avoids any assumption inherent in the Enskog equation, the comparison between MD and Enskog results determines the validity and limitations of the kinetic theory. This is the main motivation of our study. Since the parameter space over which the Enskog equation is verified is quite large, the test of the kinetic theory is quite stringent. The comparison carried out here shows that the dependence of rheology on mechanical properties and state conditions obtained from the Enskog kinetic theory presents good agreement with MD simulations, except at high density and strong dissipation. In addition, the agreement between kinetic theory and simulation results is better than the one previously reported for the homogeneous cooling state [20].

It must be noted that our analysis is restricted to the *uniform* shear flow without paying attention to the possible formation of particle clusters (microstructure). Both, kinetic theory and DSMC results intrinsically assume homogeneity, whereas in MD some degrees of inhomogeneity in density, temperature or shear rate can evolve in a steady state [45]. This can be a possible source of discrepancies between the Enskog results and MD simulations. However, in the USF problem, due to the viscous heating, inhomogeneities are weaker than for free cooling systems where clusters continuously grow in size. This is perhaps the main reason for which the results found here for a sheared (driven) fluid compare better with MD than those obtained in the undriven case [20].

The plan of the paper is as follows. In Sec. II we review the Enskog kinetic theory for USF in the case of inelastic systems along with brief descriptions of the Monte Carlo and molecular dynamics simulation methods for the USF. The comparison between the Enskog results and MD simulations is made in Sec. III. We close the paper in Sec. IV with a brief discussion of the results presented in this paper.

II. ENSKOG KINETIC THEORY AND SIMULATION METHODS

We consider a binary mixture of smooth hard spheres ($d = 3$) or disks ($d = 2$) of diameters σ_1 and σ_2, and masses m_1 and m_2. The collisions between particles of different species are characterized by three independent (constant) coefficients of normal restitution α_{11}, α_{22}, and $\alpha_{12} = \alpha_{21}$, with values $0 < \alpha_{ij} \leq 1$, where α_{ij} refers to collisions between particles of species i and j. Let us assume that the mixture is under uniform shear flow (USF). From a macroscopic point of view, the USF is characterized by a linear velocity profile

$$\mathbf{u} = ay\widehat{\mathbf{x}}, \quad a = \frac{\partial u_x}{\partial y} = \text{const.}, \tag{1}$$

where a is the (constant) shear rate and $\mathbf{u}$ refers to the (common) flow velocity. In addition, the partial densities of each species n_i and the granular temperature T are uniform, while the mass and heat fluxes vanish by symmetry reasons. The rheological properties of the system are given from the pressure tensor P, which is the only relevant flux of the problem. According to the energy balance equation, the temperature changes in time due to the competition between two mechanisms: on the one hand, viscous (shear) heating and, on the other hand, energy dissipation in collisions. In the steady state, both mechanisms cancel each other and the (steady) temperature is obtained by equating the production term due to shear work with collisional dissipation:

$$aP_{xy} = -\frac{d}{2}nT\zeta. \tag{2}$$

Here, P_{xy} denotes the xy element of the pressure tensor, $n = n_1 + n_2$ is the total number density and ζ is the cooling rate due to collisions among all the species. This steady shear flow state is what we want to analyze here.

The balance equation (2) shows the intrinsic connection between the shear field and dissipation in the system. This is a peculiar feature of granular fluids since there is an internal mechanism for which the collisional cooling sets the strength of the velocity gradient. This contrasts with the description of USF for elastic fluids where a steady state is not possible unless an external thermostat is introduced [40]. Therefore, for given values of the parameters of the mixture, in the steady state the reduced shear rate (which is the relevant nonequilibrium parameter of the problem) $a^* \propto a/\sqrt{T}$ is a function of the coefficients of restitution α_{ij} only [37]. In particular, the *quasielastic* limit ($\alpha \to 1$) naturally implies the limit of *small* shear rates ($a^* \ll 1$) and vice versa. Since the limit of small shear rates also implies a continuum-level description of the Enskog kinetic equation at the Navier-Stokes order, we may conclude that in the USF the full nonlinear dependence of the shear viscosity on the shear rate cannot be obtained from the Navier-Stokes approximation, at least for finite dissipation [37]. We shall come back to this point while discussing our results.

At a microscopic level, the USF is generated by Lees-Edwards boundary conditions [38, 39] which are simply periodic boundary conditions in the local Lagrangian frame $\mathbf{V} = \mathbf{v} - \mathsf{a}\cdot\mathbf{r}$ and $\mathbf{R} = \mathbf{r} - \mathsf{a}\cdot\mathbf{r}t$. Here, a is the tensor with elements $a_{k\ell} = a\delta_{kx}\delta_{\ell y}$. In terms of the above variables, the one-particle velocity distribution functions $f_i(\mathbf{V})$ ($i = 1, 2$) are uniform [41] and the Enskog equation takes the form

$$aV_y\frac{\partial}{\partial V_x}f_i = \sum_{j=1}^{2} J_{ij}^{\mathrm{E}}\left[\mathbf{V}|f_i,f_j\right] \ , \tag{3}$$

where the Enskog collision operator $J_{ij}^{\mathrm{E}}\left[\mathbf{V}|f_i,f_j\right]$ reads [31]

$$\begin{aligned} J_{ij}^{\mathrm{E}}\left[\mathbf{V}_1|f_i,f_j\right] \ &= \ \sigma_{ij}^{d-1}\chi_{ij}\int d\mathbf{V}_2\int d\widehat{\boldsymbol{\sigma}}\,\Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}) \\ &\times\left[\alpha_{ij}^{-2}f_i(\mathbf{V}_1')f_j(\mathbf{V}_2'+a\sigma_{ij}\widehat{\sigma}_y\widehat{\mathbf{x}}) - f_i(\mathbf{V}_1)f_j(\mathbf{V}_2 - a\sigma_{ij}\widehat{\sigma}_y\widehat{\mathbf{x}})\right]. \end{aligned} \tag{4}$$

Here, $\boldsymbol{\sigma}_{ij} = \sigma_{ij}\widehat{\boldsymbol{\sigma}}$, with $\sigma_{ij} = (\sigma_i+\sigma_j)/2$ and $\widehat{\boldsymbol{\sigma}}$ is a unit vector directed along the line of centers from the sphere of species i to the sphere of species j upon collision (i.e. at contact). In addition, Θ is the Heaviside step function, and $\mathbf{g} = \mathbf{V}_1 - \mathbf{V}_2$. The primes on the velocities denote the initial values $\{\mathbf{V}_1', \mathbf{V}_2'\}$ that lead to $\{\mathbf{V}_1, \mathbf{V}_2\}$ following a binary collision:

$$\mathbf{V}_1' = \mathbf{V}_1 - \mu_{ji}\left(1+\alpha_{ij}^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})\widehat{\boldsymbol{\sigma}}, \quad \mathbf{V}_2' = \mathbf{V}_2 + \mu_{ij}\left(1+\alpha_{ij}^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})\widehat{\boldsymbol{\sigma}}, \tag{5}$$

where $\mu_{ij} = m_i/(m_i+m_j)$. In addition, we have taken into account that the pair correlation function χ_{ij} is uniform in the USF problem. The expression for the pressure tensor P contains both *kinetic* and *collisional* transfer contributions, i.e.,

$$\mathsf{P} = \mathsf{P}^{\mathrm{k}} + \mathsf{P}^{\mathrm{c}}. \tag{6}$$

The kinetic part is given by

$$\mathsf{P}^{\mathrm{k}} = \sum_{i=1}^{2}\int d\mathbf{v}\, m_i\mathbf{V}\mathbf{V}\, f_i(\mathbf{v}), \tag{7}$$

while the collisional part is [31]

$$\begin{aligned} \mathsf{P}^{\mathrm{c}} \ &= \ \frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2}\frac{m_im_j}{m_i+m_j}\chi_{ij}\sigma_{ij}^{d}(1+\alpha_{ij})\int d\mathbf{V}_1\int d\mathbf{V}_2\int d\widehat{\boldsymbol{\sigma}}\,\Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})^2 \\ &\times\widehat{\boldsymbol{\sigma}}\widehat{\boldsymbol{\sigma}}f_i\left(\mathbf{V}_1 + a\sigma_{ij}\widehat{\sigma}_y\widehat{\mathbf{x}}\right)f_j(\mathbf{V}_2). \end{aligned} \tag{8}$$

The rheological properties of the mixture are obtained from the knowledge of the elements of the pressure tensor. Apart from these rheological properties, it is also interesting to get the temperature ratio T_1/T_2 where the partial temperatures T_i are defined as

$$T_i = \frac{m_i}{dn_i} \int d\mathbf{V}\, V^2 f_i(\mathbf{V}). \tag{9}$$

The deviation of T_1/T_2 from unity is a measure of the breakdown of the energy equipartition [18]. Finally, the cooling rate ζ is given by [31]

$$\begin{aligned}\zeta \;=\; & \frac{1}{2d}\frac{1}{nT}\sum_{i=1}^{2}\sum_{j=1}^{2}\frac{m_i m_j}{m_i+m_j}\chi_{ij}\sigma_{ij}^{d-1}(1-\alpha_{ij}^2)\int d\mathbf{V}_1\int d\mathbf{V}_2\int d\widehat{\boldsymbol{\sigma}}\,\Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})^3 \\ & \times f_i\left(\mathbf{V}_1 + a\sigma_{ij}\widehat{\sigma}_y\widehat{\mathbf{x}}\right) f_j(\mathbf{V}_2). \end{aligned} \tag{10}$$

A. Enskog simulation Monte Carlo method for USF

Needless to say, it becomes prohibitively difficult to solve analytically the Enskog equation (3) for arbitrary dissipation. As said in the Introduction, a recent approximate solution to (3) has been proposed [32]. This solution, which is based on a generalization of the Grad method, leads to a closed set of equations for the elements of the pressure tensor. However, these equations are too complicated to be useful as a practical tool in general. As an alternative to the above analytical method, an extension of the Direct Simulation Monte Carlo (DSMC) method [33] to dense gases [34, 35, 36] has been used to numerically solve (3). This method is usually referred to as the Enskog Simulation Monte Carlo (ESMC) method. This procedure was devised to mimic the dynamics involved in the Enskog collision term (still assuming operator-splitting and molecular chaos), and it has been compared to hard sphere simulations in vibrated and freely cooling systems [9, 35] and more previously has been used to analyze rheological properties of monocomponent systems for both the elastic [34] and the inelastic [19, 42] case. For a detailed description of the method applied to inelastic systems, we refer to the reader to Refs. [19] and [31].

From the simulations, one evaluates the kinetic (7) and collisional (8) contributions to the pressure tensor,

$$\mathsf{P}^{\mathrm{k}} = \sum_{i=1}^{2}\frac{m_i n_i}{N_i}\sum_{k=1}^{N_i}\mathbf{V}_k\mathbf{V}_k\ , \tag{11}$$

and

$$\mathsf{P}^{\mathrm{c}} = \frac{n}{2N\Delta t}\sum_{k\ell}^{\dagger}\frac{m_i m_j}{m_i+m_j}\sigma_{ij}(1+\alpha_{ij})(\mathbf{g}_{k\ell}\cdot\widehat{\boldsymbol{\sigma}}_{k\ell})\widehat{\boldsymbol{\sigma}}_{k\ell}\widehat{\boldsymbol{\sigma}}_{k\ell}\ , \tag{12}$$

where N_i is the number of "simulated" particles of species i, $N = N_1 + N_2$ is the total number, Δt is the time step, and the dagger (†) means that the summation is restricted to the accepted collisions. In addition, k denotes a particle of species i and ℓ a particle of species j. To improve the statistics, the results are averaged over a number $\mathcal{N}$ of independent realizations or replicas. In our simulations we have typically taken a total number of particles $N = N_1+N_2 = 10^5$, a number of replicas $\mathcal{N} = 10$, and a time step $\Delta t = 3\times10^{-3}\lambda_{11}/V_{01}(0)$. Here, $\lambda_{11} = (\sqrt{2}n_1\widetilde{\sigma}_{11})^{-1}$ is the mean free path for collisions 1–1 and $V_{01}^2(0) = 2T(0)/m_1$ where $T(0)$ is the initial temperature. Here, $\widetilde{\sigma}_{ij}$ means the total cross-section for collisions of type i–j [43]. More technical details on the application of the ESMC method to USF can be found in Ref. [31].

In the simulations the initial velocity distribution function is that of local equilibrium. The ESMC simulation is prepared as follows: after an initial transient period, the system reaches a steady state where the values obtained for the reduced quantities, see below Eqs. (13)–(15), are independent of the initial preparation of the system. Their values do depend on the values of the coefficients of restitution, the packing fraction, and the ratios of mass, concentrations and sizes.

B. Event-driven simulation method for uniform shear flow

The molecular dynamics (MD) and event-driven (ED) simulation methods are extensively discussed, e.g. in textbooks [38], for elastic systems, and were also applied to sheared granular systems, see Refs. [23], [25], [44], [45] and references therein. Also the preparation-procedure and system size dependences are discussed in Ref. [23] with no striking insights, so that we do not repeat these details here.

C. Rheology

The rheological properties of the mixture are determined from the nonzero elements of the pressure tensor. Possibilities to non-dimensionalize are to scale either by the relevant small species contributions [23] or by the corresponding mean values [44]. Applying the former scheme, one arrives at the reduced shear viscosity

$$\mu = \frac{|P_{xy}|}{\varrho_1 \sigma_1^2 a^2}, \tag{13}$$

the reduced temperature

$$\theta = \frac{T}{m_1 \sigma_1^2 a^2}, \tag{14}$$

and the reduced pressure

$$\Pi = \frac{p}{\varrho_1 \sigma_1^2 a^2}, \quad p = \frac{1}{d} \mathrm{tr}\, \mathsf{P}. \tag{15}$$

Here $\mathrm{tr}\, \mathsf{P}$ denotes the trace of the pressure tensor P and ϱ_i is the material density of species i. In the case of hard disks $\varrho_i = 4m_i/\pi\sigma_i^2$ while $\varrho_i = 6m_i/\pi\sigma_i^3$ for hard spheres.

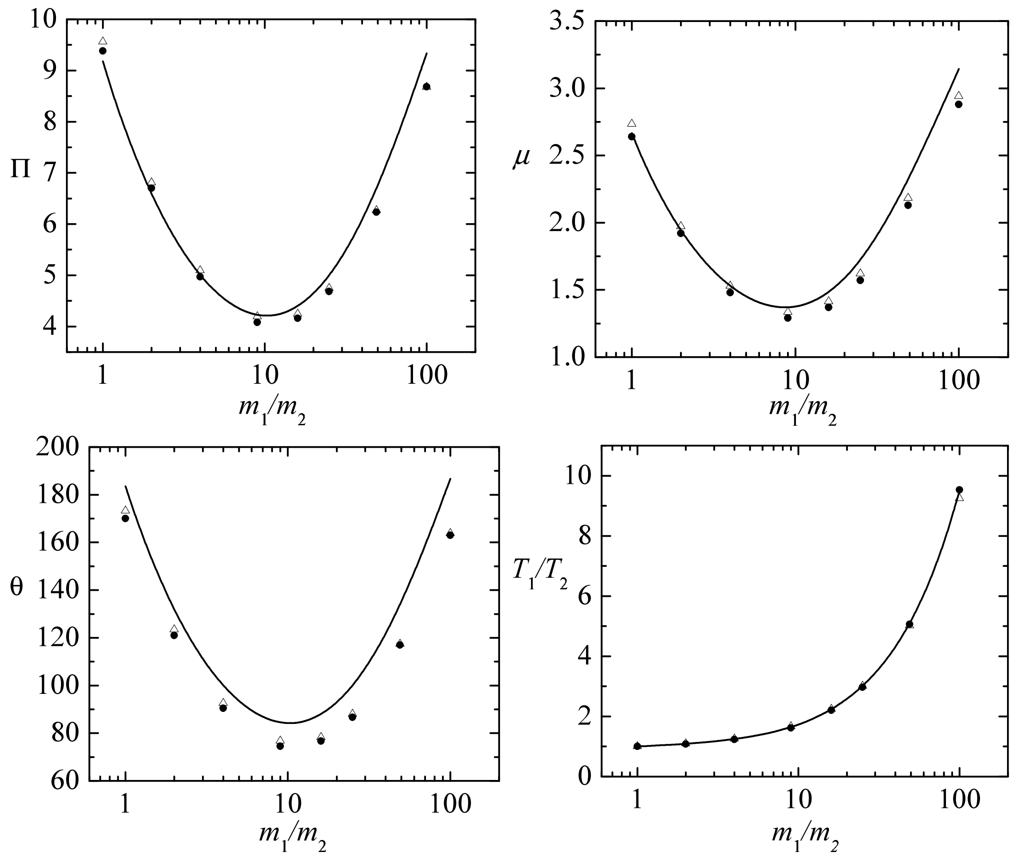

FIG. 1: Reduced pressure Π, reduced shear viscosity μ, reduced temperature θ and temperature ratio T_1/T_2 plotted against the mass ratio m_1/m_2 for an equimolar mixture ($x_1 = \frac{1}{2}$) of hard disks ($d = 2$) with $\sigma_1/\sigma_2 = 1$, $\phi = 0.05$ and $\alpha = 0.9$. The lines are the analytical results obtained from the Boltzmann kinetic equation while the symbols correspond to the ESMC results (circles) and MD simulations (triangles).

As said before, in the steady state and for given values of the parameters of the mixture, the (dimensionless) rheological properties μ, θ, and Π are functions of the coefficients of restitution α_{ij} only, and their dependences on the shear-rate are scaled out. The parameters of the mixture are the mass ratio m_1/m_2, the mole fraction $x_1 = n_1/n$,

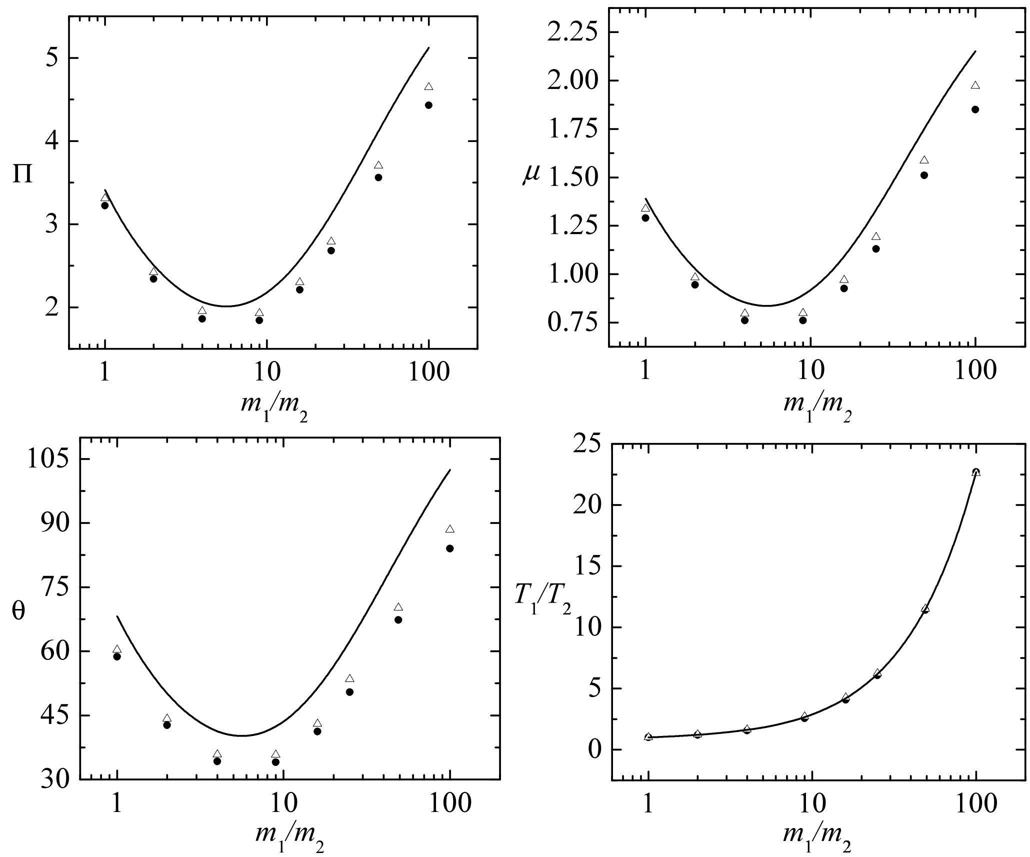

FIG. 2: The same as Fig. 1, only with $\alpha = 0.75$. Note the different axis scaling as compared to Fig. 1.

the ratio of diameters σ_1/σ_2, and the total solid volume fraction $\phi = \phi_1 + \phi_2$ where $\phi_i = n_i m_i/\varrho_i$ is the species volume fraction of the component i. In the following, our aim is to examine the dependence of μ, θ, Π, and T_1/T_2 on dissipation as well as on the parameters of the mixture, and make a detailed comparison between theory and simulations.

III. RESULTS

A. 2D results

The main objective of this Section is to compare the results obtained from the ESMC method with those obtained from MD simulations performed for bidisperse mixtures of smooth hard disks ($d = 2$). For the sake of simplicity, we assume that all the coefficients of restitution are set equal ($\alpha_{ij} \equiv \alpha$) so that the parameter space of the problem is reduced to five quantities: $\{\alpha, \phi, m_1/m_2, \sigma_1/\sigma_2, x_1\}$, where $m_1 \geq m_2$ and $\sigma_1 \geq \sigma_2$ is implied in the following.

For the pair correlation function values at contact, χ_{ij}, the relation [46]

$$\chi_{ij} = \frac{1}{1-\phi} + \frac{9}{16}\frac{\beta}{(1-\phi)^2}\frac{\sigma_i\sigma_j}{\sigma_{ij}}, \tag{16}$$

is used in the Enskog and ESMC calculations, where $\beta = \pi(n_1\sigma_1 + n_2\sigma_2)/4$. The approximation (16) for the equilibrium pair correlation function is accurate in most of the fluid region, although a more detailed comparison with computer simulations shows that the expression becomes less accurate with increasing density and diameter ratios [47]. However, given the values considered in our simulations, we expect that these approximations to χ_{ij} turn out to be reliable with an error margin of much less than one per-cent, so that we do not consider the higher order corrections here.

Three different values of the solid volume fraction ϕ have been considered here, $\phi = 0.05$, $\phi = 0.1$, and $\phi = 0.2$. The first value of ϕ represents a dilute gas while the two latter can be considered as moderately dense fluids. To

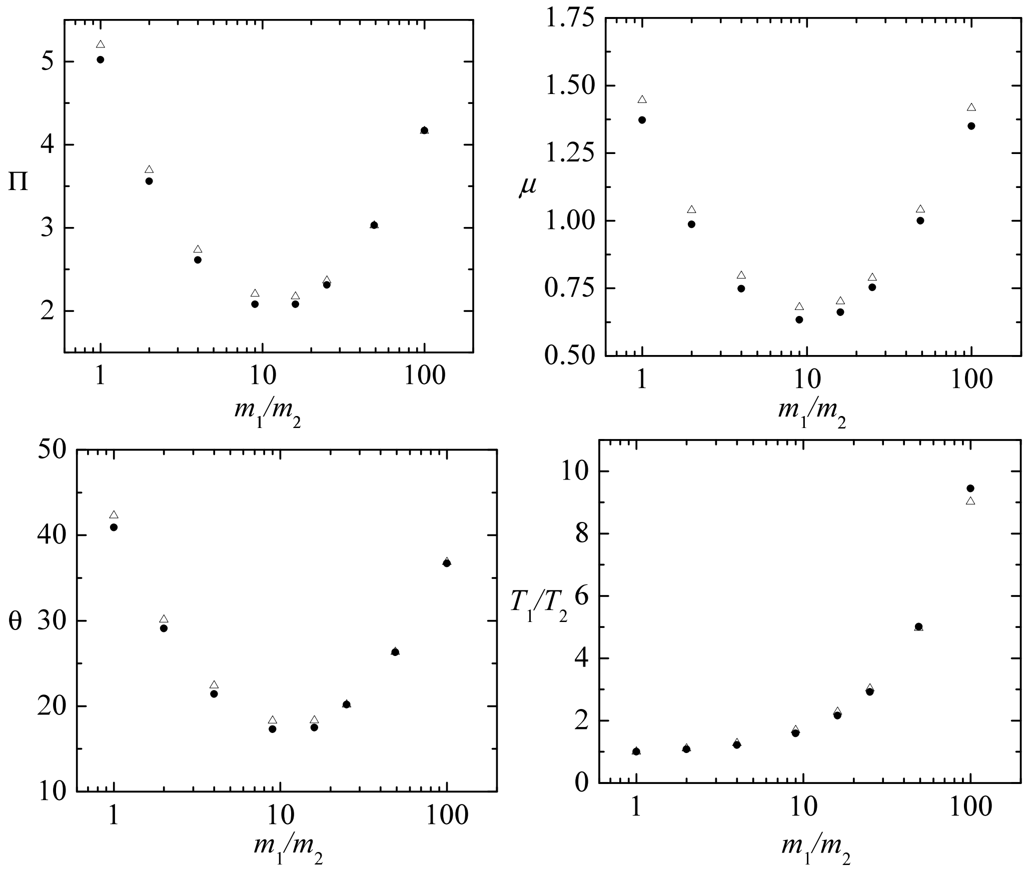

FIG. 3: The same as Fig. 1, only with $\phi = 0.1$.

compare with MD results, two values of the coefficient of restitution have been considered, $\alpha = 0.9$ and $\alpha = 0.75$, both representing moderately strong dissipation. We have taken an equimolar mixture ($x_1 = \frac{1}{2}$) with particles of equal size ($\sigma_1 = \sigma_2$) but with quite different masses. Specifically, we have studied the dependence of μ, θ, Π, and the temperature ratio T_1/T_2 on the mass ratio m_1/m_2 for different values of α and ϕ. As said before, as the coefficient of restitution decreases, the system goes away from equilibrium and the energy equipartition is not expected to hold.

In Figs. 1 and 2, we plot Π, μ, θ, and T_1/T_2 against m_1/m_2 for low density, $\phi = 0.05$, and the coefficients of restitution $\alpha = 0.9$ and $\alpha = 0.75$, respectively. The symbols refer to MD simulations (triangles) and ESMC results (circles) while the solid lines correspond to the results obtained from the Boltzmann equation [31], which is strictly valid in the limit $\phi \to 0$. In Fig. 1, the agreement between the ESMC and MD results is excellent, even for very disparate masses. The Boltzmann results compare also quite well with simulations, especially in the case of the temperature ratio. For the steady temperature, the Boltzmann predictions slightly overestimate the MD simulation results. These discrepancies can be primarily attributed to density effects, since previous comparisons between theory and DSMC results show better agreement for $\phi = 0$ than the one reported here [29]. Comparing the two figures, one can conclude that the agreement between the Boltzmann kinetic theory and the simulation data becomes worse with increasing dissipation. The only exception is the temperature ratio which is essentially obtained from the diagonal elements of the kinetic contribution to the pressure tensor. We also observe good agreement between Enskog and MD results, except for the largest values of the mass ratio.

Figures 3 and 4 depict results for the higher densities $\phi = 0.1$ and $\phi = 0.2$, with a coefficient of restitution $\alpha = 0.9$. The Enskog (ESMC) results agree well with the MD simulations, only does the discrepancy increase in general with decreasing mass ratio for the pressure Π and the temperature θ, while the opposite occurs for the temperature ratio. We also observe that in general the Enskog kinetic theory underestimates the MD results. Thus, for instance in the case $m_1/m_2 = 4$ and for $\phi = 0.2$, the discrepancies for Π, μ, T_1/T_2, and θ are about 5%, 7%, 7%, and 5%, respectively. In addition, both Enskog and MD results clearly predict a *non-monotonic* behavior of the pressure and the viscosity on the mass ratio. This conclusion contrasts with the predictions of kinetic theories [24] based on the equipartition assumption which suggest a monotonic dependence of Π and μ on m_1/m_2 [29, 44]. With respect to

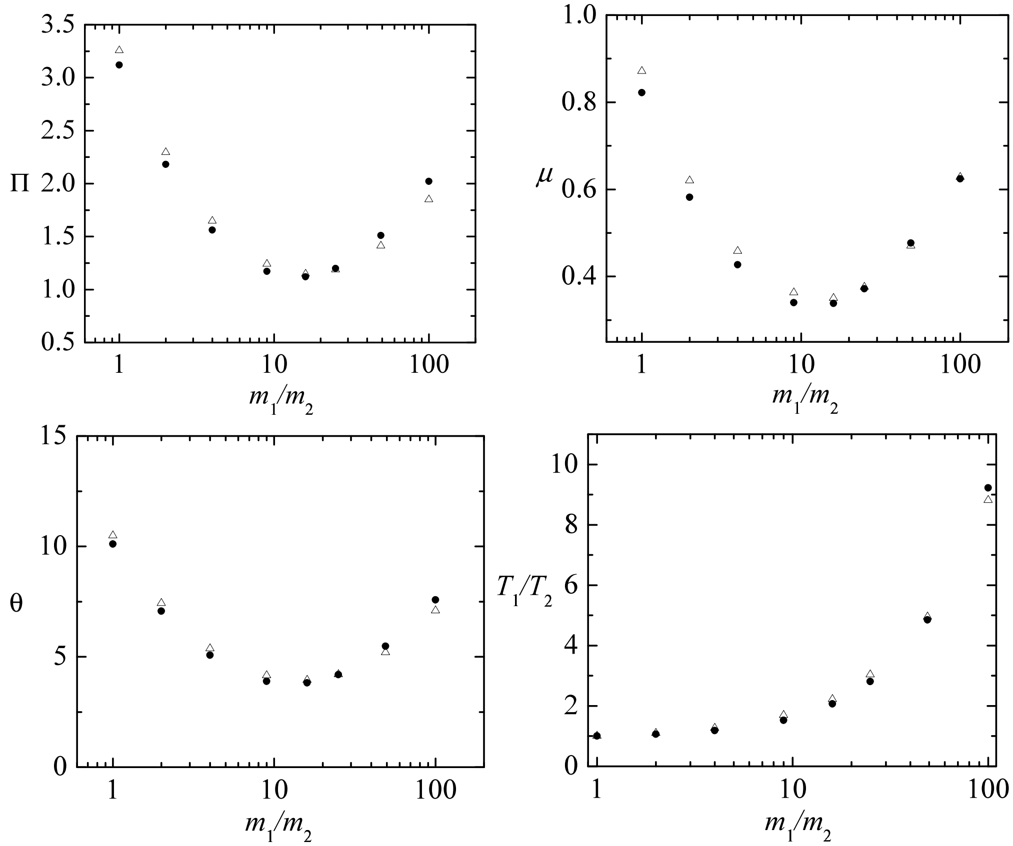

FIG. 4: The same as Fig. 1, only with $\phi = 0.2$.

the behavior of the temperature ratio, we observe that T_1/T_2 exhibits a strong dependence on the mass ratio. The mass disparity enhances the magnitude of the non-equipartition of energy. Differences between the Enskog theory and MD simulations become more significant as the dissipation increases, as shown in Fig. 5 for $\phi = 0.2$ and $\alpha = 0.75$. Although the Enskog theory captures well the trends observed in MD simulations, the disagreement between both approaches is more important than the one observed in previous cases. More specifically, in the case $m_1/m_2 = 4$, the discrepancies for Π, μ, T_1/T_2, and θ are now about 9%, 6%, 11%, and 10%, respectively. However, given that these deviations are not quite large, one can still consider the Enskog equation as a good approximation for describing the rheological properties of a granular mixture, even for moderately high density and strong dissipation.

B. 3D results

In the case of hard spheres ($d = 3$), we take for the pair correlation function χ_{ij} the following approximation [48]

$$\chi_{ij} = \frac{1}{1-\phi} + \frac{3}{2}\frac{\beta}{(1-\phi)^2}\frac{\sigma_i\sigma_j}{\sigma_{ij}} + \frac{1}{2}\frac{\beta^2}{(1-\phi)^3}\left(\frac{\sigma_i\sigma_j}{\sigma_{ij}}\right)^2, \tag{17}$$

where now $\beta = \pi(n_1\sigma_1^2 + n_2\sigma_2^2)/6$. We compare the ESMC and ED results obtained for a mixture under USF with a kinetic theory recently proposed [31]. In contrast to previous theories [24, 25], the above theory takes into account the effect of non-equipartition of granular energy on the transport coefficients. This theory is based on the Chapman-Enskog solution [30] to the Enskog equation in the first order of the shear rate (Navier-Stokes approximation). However, given that USF is inherently non-Newtonian, the full nonlinear dependence of the viscosity on the shear rate is required. This implies that there is no possibility *a priori* of using the Navier-Stokes equations to describe the (shear-rate dependent) rheological properties of USF, especially as the dissipation increases [37]. In Fig. 6 we plot the reduced quantities Π, μ, θ, and T_1/T_2 as a function of the coefficient of restitution α for $\sigma_1/\sigma_2 = 1$, $x_1 = \frac{1}{2}$, $m_1/m_2 = 4$, and $\phi = 0.1$ as given by Monte Carlo simulations (circles), MD simulations (triangles) and the

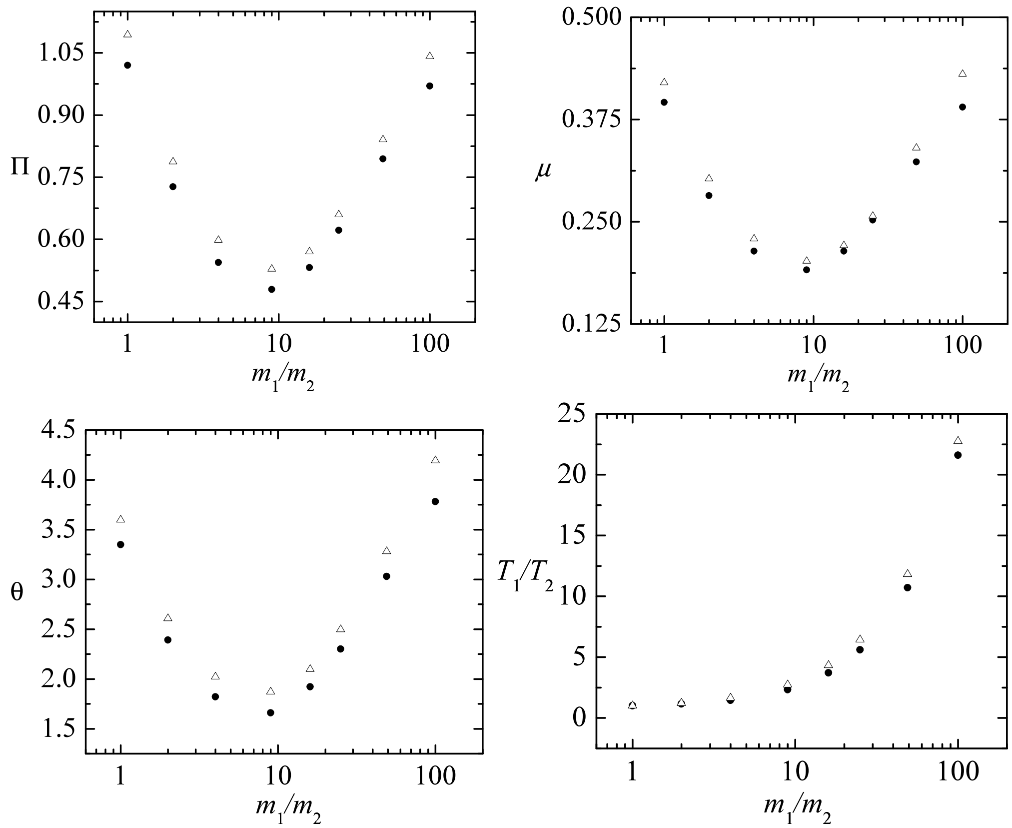

FIG. 5: The same as Fig. 1, only with $\phi = 0.2$ and $\alpha = 0.75$.

Chapman-Enskog solution (solid lines). Given that in reduced units, the shear rate and dissipation are not independent parameters, one would expect that the differences between the Navier-Stokes predictions and the simulation results increase as the coefficient of restitution decreases. Figure 6 confirms the above expectations since, for instance, the discrepancies between theory and MD simulations for Π, μ, θ, and T_1/T_2 are about 30%, 43%, 32%, and 10%, respectively, at $\alpha = 0.7$. This shows again that the hydrodynamic description of the USF state is non-Newtonian. Nevertheless, the main trends observed for the rheological properties are qualitatively well captured by the Chapman-Enskog solution. Concerning the comparison between the ESMC and MD results we observe good agreement, except for strong dissipation where the discrepancies are significant (say, for instance, about 10% for $\alpha = 0.7$).

IV. DISCUSSION

In an effort to validate the Enskog kinetic theory, the Enskog equation for a binary mixture of smooth *inelastic* hard disks/spheres under uniform shear flow (USF), in steady state, has been numerically solved by means of the ESMC method [34]. This method can be considered as the extension of the well-known DSMC method [33] of the Boltzmann equation for finite densities. Results for the (reduced) rheological properties and the temperature ratio have been reported in a wide parameter space (mass ratio, density, and coefficients of restitution). Variations of the diameter ratio and the composition were studied elsewhere [23]. In addition, the ESMC results have been compared to event-driven molecular dynamics (MD) for hard disks/spheres as well as to solutions of the Boltzmann equation in the low density limit [19] and of the Enskog equation for small shear rates [31].

We have considered mixtures constituted by particles of equal size and have basically focused on studying the effect of mass disparity on the rheological behavior of sheared 2D granular mixtures and the effect of dissipation on the rheological behavior of sheared 3D granular mixtures. For the 2D simulations, three different values for the solid volume fraction (ϕ=0.05, 0.1, and 0.2) and two values of the coefficient of restitution (α=0.9 and 0.75) were considered. In the case of α=0.9, the comparison shows that there are no significant qualitative differences between the results obtained from MD simulations and those that follow from the ESMC method. As the dissipation increases

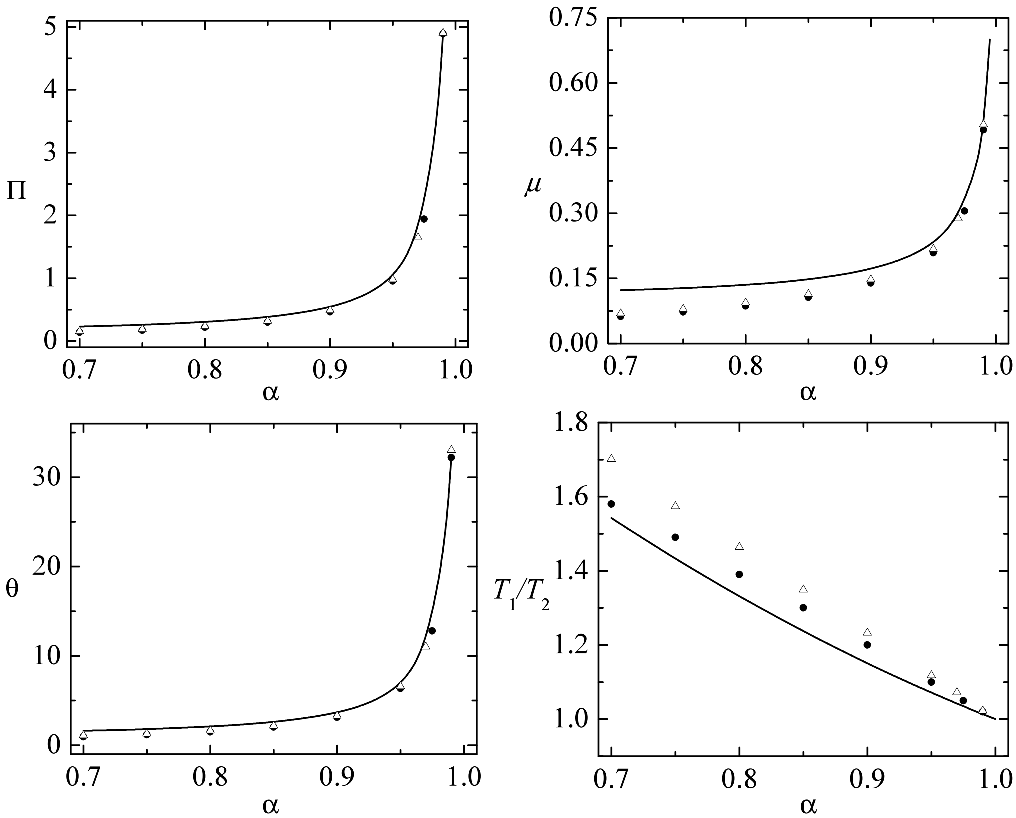

FIG. 6: Plot of the reduced pressure Π, the reduced shear viscosity μ, the reduced temperature θ and the temperature ratio T_1/T_2 versus the coefficient of restitution α for an equimolar mixture ($x_1 = \frac{1}{2}$) of hard spheres ($d = 3$) with $\sigma_1/\sigma_2 = 1$, $m_1/m_2 = 4$, and $\phi = 0.1$. The lines are the analytical results obtained from the Chapman-Enskog solution up to the Navier-Stokes order while the symbols (circles) correspond to the ESMC results.

($\alpha = 0.75$), although the Enskog predictions compare qualitatively well with MD data, the discrepancies between both approaches become more prominent. These discrepancies tend to increase also with increasing density. On the other hand, the good agreement found here includes densities well outside of the Boltzmann limit and values of dissipation that clearly lie outside of what can be considered the quasielastic limit. This test may be taken again as a further testimony to the usefulness of the Enskog equation for fluids with elastic and inelastic collisions, including mixtures.

Like the Boltzmann equation, the Enskog kinetic theory [19, 31] assumes the molecular chaos hypothesis and thus the two particle velocity correlations for a pair of particles at contact are neglected. However, as mentioned in the Introduction, recent MD simulations performed in the homogeneous case for driven [10, 11, 12] and for undriven [13] granular gases have observed velocity correlations for pairs of particles that are about to collide. These short-range velocity correlations were relevant for high densities and finite dissipation. Consequently, some disagreement between the Enskog theory and simulations with increasing dissipations is expected. However, the magnitude of disagreement with increasing dissipation is not much, and hence the validity of the Enskog kinetic theory appears to span a much wider range than the limit of nearly elastic collisions. On the other hand, the failure of the Enskog kinetic theory at high densities is expected just as for fluids with elastic collisions [50]. This is possibly due to multiparticle collisions, including recollision events (ring collisions).

There is some indication that the effects of correlated collisions are enhanced at strong dissipation since the colliding particles tend to become more focused [10, 11, 12]. Furthermore, our results also indicate that the range of densities for which the Enskog equation holds decreases with increasing dissipation. This conclusion agrees with previous findings made for mixtures in the homogeneous cooling state [20] and for the case of the self-diffusion coefficient [51]. The specific mechanism responsible for these discrepancies at higher densities and its quantitative prediction remains an open problem.

As said in the Introduction, one possible source of discrepancies observed between Enskog results and MD simulations is due to the fact that while theory and ESMC results are restricted to a homogeneous state (in the Lagrangian frame), some degree of inhomogeneity (especially for density) evolves in MD simulations in the steady state. However,

in a *driven* (sheared) system inhomogeneities are weaker than for *free* cooling systems where clusters grow and grow without being disturbed by the action of the energy input. For this reason, the magnitude of the differences between the Enskog predictions and MD simulations observed here are in general smaller than those previously reported in the undriven homogeneous case [20, 51] for the same values of density and coefficients of restitution. In this context, it could be said that the range of densities and dissipation for which the Enskog kinetic theory applies depends rather strongly on the state of the system, and cannot be given as a general rule. In the USF problem considered here, it seems that the Enskog equation can be taken as a reliable model to get the dependence of the rheological properties on the mechanical parameters of the mixture.

Nevertheless, the (steady) USF problem is inherently non-Newtonian [37, 45]. Due to the coupling between the reduced shear rate (measured through the reduced temperature θ) and dissipation, large gradients can occur as the system becomes more inelastic. This implies that the shear viscosity coefficient in USF cannot be deduced from the usual Navier-Stokes or Newtonian hydrodynamic equations (which are linear in the gradients) [37]. The comparison carried out in Fig. 6 in the case of hard spheres shows that the Navier-Stokes predictions obtained from a recent Chapman-Enskog solution [28] deviate from the ESMC results obtained for USF as the coefficient of restitution decreases. However, the agreement found between theory and Monte Carlo simulations extends beyond the quasielastic limit (say for instance, for $\alpha \simeq 0.97$), except for the temperature ratio. In this sense, it is possible that the failure of the Navier-Stokes approximation to describe non-Newtonian properties could be in part mitigated by the introduction of appropriate reduced quantities, such as those defined by Eqs. (13)–(15).

Given that the dynamical velocity correlations measured in previous works [10, 11, 12] become important as the fluid density increases, some authors [10, 13] conclude that the Enskog equation can be insufficient to compute average properties of the fluid. This conclusion contrasts with the results reported in this paper where, at least for the problem studied here, velocity correlations do not seem to play a relevant role and the Enskog equation accurately predicts the rheological properties of the system. It is possible that for more complex situations, velocity correlations become important even before the system develops significant spatial correlations and the Enskog theory (which only takes into account spatial correlations) does not provide reliable predictions. In this case, new kinetic theories incorporating the effect of velocity correlations are needed to describe dense granular fluids at finite dissipation.

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